APPENDIX B

Definitions

Appendix B

Definitions

- **Adsorption** partitioning of a dissolved species onto a solid surface.
- **Adsorption Edge** the pH range where solute adsorption sharply changes from $\sim 10\%$ to $\sim 90\%$.
- **Actinon** name occasionally used, especially in older documents, to refer to ²¹⁹Rn which forms from the decay of actinium.
- Activity the effective concentration on an ion that determines its behavior to other ions with which it might react. An activity of ion is equal to its concentration only in infinitely dilute solutions. The activity of an ion is related to its analytical concentration by an activity coefficient, γ .
- **Alkali Metals** elements in the 1A Group in the periodic chart. These elements include lithium, sodium, potassium, rubidium, cesium, and francium.
- **Alpha Particle** particle emitted from nucleus of atom during 1 type of radioactive decay. Particle is positively charged and has 2 protons and 2 neutrons. Particle is physically identical to the nucleus of the ⁴He atom (Bates and Jackson 1980).
- **Alpha Recoil** displacement of an atom from its structural position, as in a mineral, resulting from radioactive decay of the release an alpha particle from its parent isotope (*e.g.*, alpha decay of ²²²Rn from ²²⁶Ra).
- **Amphoteric Behavior** the ability of the aqueous complex or solid material to have a negative, neutral, or positive charge.
- Basis Species see component species.

Cation Exchange - reversible adsorption reaction in which an aqueous species exchanges with an adsorbed species. Cation exchange reactions are

$$CaX(s) + {}^{90}Sr^{2+}(aq) = {}^{90}SrX(s) + Ca^{2+}(aq)$$

- approximately stoichiometric and can be written, for example, as where X designates an exchange surface site.
- Cation Exchange Capacity (CEC) the sum total of exchangeable cations per unit mass of soil/sediment that a soil can adsorb.
- Clay Content particle size fraction of soil that is less than 2 μ m (unless specified otherwise).
- **Code Verification** test of the accuracy with which the subroutines of the computer code perform the numerical calculations.
- **Colloid** any fine-grained material, sometimes limited to the particle-size range of <0.00024 mm (*i.e.*, smaller than clay size), that can be easily suspended. In its original sense, the definition of a colloid included any fine-grained material that does not occur in crystalline form.
- **Complexation (Complex Formation)** any combination of dissolved cations with molecules or anions containing free pairs of electrons.
- **Component Species** "basis entities or building blocks from which all species in the system can be built" (Allison *et al.*, 1991). They are a set of linearly independent aqueous species in terms of which all aqueous speciation, redox, mineral, and gaseous solubility reactions in the MINTEQA2 thermodynamic database are written.
- **Detrital Mineral** "any mineral grain resulting from mechanical disintegration of parent rock" (Bates and Jackson 1980).
- **Deuterium (D)** stable isotopes ²H of hydrogen.
- **Disproportionation** is a chemical reaction in which a single compound serves as both oxidizing and reducing agent and is thereby converted into more oxidized and a more reduced derivatives (Sax and Lewis 1987). For the reaction to occur, conditions in the system must be temporarily changed to favor this

reaction (specifically, the primary energy barrier to the reaction must be lowered). This is accomplished by a number of ways, such as adding heat or microbes, or by radiolysis occurring. Examples of plutonium disproportionation reactions are:

$$3Pu^{4+} + 2H_2O = 2Pu^{3+} + PuO_2^{2+} + 4H^+$$

$$3PuO_2^+ + 4H^+ = Pu^{3+} + 2PuO_2^{2+} + 2H_2O.$$

Electron Activity - unity for the standard hydrogen electrode.

Far Field - the portion of a contaminant plume that is far from the point source and whose chemical composition is not significantly different from that of the uncontaminated portion of the aquifer.

Fulvic Acids - breakdown products of cellulose from vascular plants (also see humic acids). Fulvic acids are the alkaline-soluble portion which remains in solution at low pH and is of lower molecular weight (Gascoyne 1982).

Humic Acids - breakdown products of cellulose from vascular plants (also see fulvic acids). Humic acids are defined as the alkaline-soluble portion of the organic material (humus) which precipitates from solution at low pH and are generally of high molecular weight (Gascoyne 1982).

Hydrolysis - a chemical reaction in which a substance reacts with water to form 2 or more new substances. For example, the first hydrolysis reaction of U⁴⁺ can be written as

$$U^{4+} + H_2O = UOH^{3+} + H^+.$$

Hydrolytic Species - an aqueous species formed from a hydrolysis reaction.

Ionic Potential - ratio (z/r) of the formal charge (z) to the ionic radius (r) of an ion.

Isoelectric Point (iep) - pH at which a mineral's surface has a net surface charge of zero. More precisely, it is the pH at which the particle is electrokinetically uncharged.

Lignite - a coal that is intermediate in coalification between peat and

subbituminous coal.

Marl - an earthy substance containing 35-65% clay and 65-35% carbonate formed under marine or freshwater conditions

Mass Transfer - transfer of mass between 2 or more phases that includes an aqueous solution, such as the mass change resulting from the precipitation of a mineral or adsorption of a metal on a mineral surface.

Mass Transport - time-dependent movement of 1 or more solutes during fluid flow.

Mire - a small piece of marshy, swampy, or boggy ground.

Model Validation - integrated test of the accuracy with which a geochemical model and its thermodynamic database simulate actual chemical processes.

Monomeric Species - an aqueous species containing only 1 center cation (as compared to a polymeric species).

Near Field - the portion of a contaminant plume that is near the point source and whose chemical composition is significantly different from that of the uncontaminated portion of the aquifer.

Peat - an unconsolidated deposit of semicarbonized plant remains in a water saturated environment.

Polynuclear Species - an aqueous species containing more than 1 central cation moiety, e.g., $(UO_2)_2CO_3(OH)_3^2$ and $Pb_4(OH)_4^{4+}$.

Protium (H) - stable isotope ¹H of hydrogen.

Retrograde Solubility - solubility that decreases with increasing temperature, such as those of calcite (CaCO₃) and radon. The solubility of most compounds (*e.g.*, salt, NaCl) increases with increasing temperature.

Species - actual form in which a dissolved molecule or ion is present in solution.

Specific Adsorption - surface complexation via a strong bond to a mineral surface.

For example, several transition metals and actinides are specifically adsorbed to aluminum- and iron-oxide minerals.

Sol - a homogeneous suspension or dispersion of colloidal matter in a fluid.

Solid Solution - a solid material in which a minor element is substituted for a major element in a mineral structure.

Thoron - name occasionally used, especially in older documents, to refer to ²²⁰Rn which forms from the decay of thorium.

Tritium (T) - radioactive isotope ³H of hydrogen.

Tritium Units - units sometimes used to report tritium concentrations. A tritium unit (TU) is equivalent to 1 atom of ³H (tritium) per 10¹⁸ atoms of ¹H (protium). In natural water that produces 7.2 x 10⁻³ disintegrations per minute per milliliter (dpm/ml) of tritium, 1 TU is approximately equal to 3.2 picocuries/milliliter (pCi/ml).